

# ABSENCE OF A GROUND STATE FOR BOSONIC COULOMB SYSTEMS WITH CRITICAL CHARGE

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**ABSTRACT.** We consider bosonic Coulomb systems with  $N$ -particles and  $K$  static nuclei. Let  $E_N^Z$  denote the ground state energy of a bosonic molecule of the total nuclear charge  $Z$ . We prove that the system has no normalizable ground state when  $E_N^{N-1} = E_{N-1}^{N-1}$ .

## 1. INTRODUCTION

We consider a molecule consisting of  $N$ -particles and  $K$  fixed nuclei with positive charges  $z_1, \dots, z_K > 0$  located at distinct positions  $R_1, \dots, R_K \in \mathbb{R}^3$ . Let  $Z = \sum_{i=1}^K z_i$  be the total nuclear charge. This system is described by the Hamiltonian

$$H_N^Z = \sum_{i=1}^N \left( -\Delta_i - \sum_{j=1}^K z_j |x_i - R_j|^{-1} \right) + \sum_{1 \leq i < j \leq N} |x_i - x_j|^{-1} + \sum_{1 \leq i < j \leq K} z_i z_j |R_i - R_j|^{-1}$$

acting on  $L^2(\mathbb{R}^{3N})$ . Here  $x_i$ 's in  $\mathbb{R}^3$  and  $\Delta_i$  are, respectively, the particle coordinates and the three-dimensional Laplacian with respect to the coordinate  $x_i$ . It is well-known that  $H_N^Z$  is a self-adjoint operator with the domain  $H^2(\mathbb{R}^{3N})$ , and bounded from below. The ground state energy is defined by

$$E_N^Z = \inf \text{spec } H_N^Z = \inf \{ \langle \psi, H_N^Z \psi \rangle : \psi \in H^1(\mathbb{R}^{3N}), \|\psi\|_2 = 1 \}$$

and if it is an eigenvalue, the corresponding eigenfunction is called the ground state. It is always the case that  $E_N^Z \leq E_{N-1}^Z$  (see, e.g., [12]).

According to the HVZ theorem ([12]),  $E_N^Z < E_{N-1}^Z$  implies that there exists a ground state eigenfunction of  $H_N^Z$ . Zhislin [18] proved that  $E_N^Z < E_{N-1}^Z$  for  $Z > N - 1$  and it is also known that the system is not bound for all small  $Z$  compared to  $N$ . More precisely, the system has no ground state if  $N \geq 2Z + K$  ([14]). This implies instability of the di-anion  $\text{H}^{2-}$ . In the usual fermionic case, it is believed that there are no atomic long-lived di-anions  $\text{X}^{2-}$ , i.e., fermionic atoms are not bound if  $N > Z + 1$  (see, [16] for further information).

In the critical case  $Z = N - 1$ , it might happen either  $E_N^{N-1} < E_{N-1}^{N-1}$  or  $E_N^{N-1} = E_{N-1}^{N-1}$ . The latter case leads to absence of anions (e.g., presumably,  $\text{He}^-$ ,  $\text{Be}^-$ , etc) or, otherwise, existence of bound states having zero binding energy as well [8, 3, 7]. In

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this paper, we prove that the ground states of bosonic molecules are delocalized when  $E_N^{N-1} = E_{N-1}^{N-1}$ .

**Theorem 1.1.** *Suppose  $E_N^{N-1} = E_{N-1}^{N-1}$ . Then there cannot be a normalizable ground state of  $H_N^{N-1}$  in  $L^2(\mathbb{R}^{3N})$ .*

Thus, bosonic anions  $X^-$  fail to be stable in that case. In nature, fermionic  $\text{He}^-$  anion ( $N = 3, Z = 2$ ) is unstable as well as numerical evidence [6] (but a virtual state can be expected as indicated by [10]). On the other hand, Hogreve [11] proved bosonic  $\text{He}^-$  can exist as a stable anion.

For the atom with  $N = 2$  electrons,  $\text{H}^-$  anion ( $Z = 1$ ) has a ground state ([17, 5]). Moreover, for bosonic atoms it is known that  $E_N^Z < E_{N-1}^Z$  for all  $N \leq N_c(Z) = 1.21Z + o(Z)$  as  $Z \rightarrow \infty$ , where  $N_c(Z)$  is the maximum number of particles that can be bound to a nucleus of charge  $Z$  ([4, 2]). In particular,  $E_N^{N-1} < E_{N-1}^{N-1}$  for  $N$  sufficiently large.

**Remark 1.2.** Let  $Z_c > 0$  be a critical value such that for  $Z > Z_c$  one has  $E_N^Z < E_{N-1}^Z$ , and  $E_N^{Z_c} = E_{N-1}^{Z_c}$ . Clearly,  $Z_c \leq N - 1$  by Zhislin's theorem. Our theorem corresponds to the case  $Z_c = N - 1$ . In the atomic case  $K = 1$ , it was shown by [3, 7],  $H_N^{Z_c}$  has a ground state if  $Z_c < N - 1$  and  $E_{N-1}^{Z_c} < E_{N-2}^{Z_c}$  (in [7], if  $Z_c \in (N - 2, N - 1)$ ). Furthermore, these results are also valid for the fermionic case. But our proof works only for unconstrained (bosonic) case because the positivity of the ground state is needed.

## 2. PROOF OF THEOREM 1.1

Our method is similar to that of M. and T. Hoffman-Ostenhoff [9]. They showed that the Hamiltonian of the two-particle atom  $H_2^{Z_c}$  has no ground state in the triplet S-sector at the threshold  $Z_c = 1$ . The triplet S-sector means that the admissible functions in  $L^2(\mathbb{R}^6)$  are restricted to  $\psi(x_1, x_2) = -\psi(x_2, x_1)$  and  $\psi(x_1, x_2) = \psi(|x_1|, |x_2|, x_1 \cdot x_2)$ .

Our proof is simpler than the one in [9], and we treat the molecule of arbitrary  $N$ -particles, but without the anti-symmetry assumption (the Pauli exclusion principle).

Suppose indirectly that there is a  $\psi \in H^1(\mathbb{R}^{3N})$  so that  $H_N^Z \psi = E_N^Z \psi$  and  $\psi \neq 0$  for  $Z = Z_c = N - 1$ . The ground state eigenfunction  $\psi$  is automatically in  $H^2(\mathbb{R}^{3N})$ , and we may assume that  $\psi \geq 0$  ([15, Theorem 7.8]). Then, by the results of Aizenman and Simon [1, Theorem 3.10 & 1.5],  $\psi$  is strictly positive and continuous.

For any function  $g : \mathbb{R}^{3N} \rightarrow \mathbb{R}$  let

$$[g](x_1, \dots, x_{N-1}, r_N) = |\mathbb{S}^2|^{-1} \int_{\mathbb{S}^2} g(x_1, \dots, x_N) d\omega_N$$

be the spherical average of  $g$  with respect to the variable  $x_N = (r_N, \omega_N)$ , where  $d\omega_N$  is the spherical measure on  $\mathbb{S}^2$ , which is the unit sphere in  $\mathbb{R}^3$ , and  $|\mathbb{S}^2|$  is the area of  $\mathbb{S}^2$ . We note that  $\|[g]\|_2 \leq \|g\|_2$  for any  $g$  by the Cauchy-Schwarz inequality.

The next lemma is a slight modification of [13, Lemma 7.17].

**Lemma 2.1.** *Let  $\psi$  be a strictly positive, continuous function in  $H^2(\mathbb{R}^{3N})$  and set  $f = \exp([\ln \psi](x_1, \dots, x_{N-1}, r_N))$ . Then  $f > 0$ ,  $f \in C(\mathbb{R}^{3N})$ , and*

$$\left[ \frac{\Delta_i \psi}{\psi} \right] f \geq \Delta_i f \quad (i = 1, \dots, N)$$

*in the sense of distributions. Moreover,  $\nabla_i f \in L^2_{\text{loc}}(\mathbb{R}^{3N})$  and  $\Delta_i f \in L^1_{\text{loc}}(\mathbb{R}^{3N})$ , as the weak derivative, for  $i = 1, \dots, N$ .*

*Proof.* Note that  $f \leq [\psi] \in L^2(\mathbb{R}^{3N})$  from Jensen's inequality ([15, Theorem 2.2]). Let  $\rho_\varepsilon$  be a mollifier in  $\mathbb{R}^{3N}$ , namely,  $\rho_\varepsilon(x) = \varepsilon^{-3N} \rho(\varepsilon^{-1}x)$ , for  $\varepsilon > 0$ , where  $\rho$  is a function in  $C_c^\infty(\mathbb{R}^{3N})$  (infinitely differentiable functions with compact support) satisfying  $\rho \geq 0$ ,  $\int \rho = 1$ ,  $\rho(x) = 0$  for  $|x| \geq 1$ . Then  $\psi_\varepsilon = \rho_\varepsilon * \psi$  is strictly positive, smooth and satisfies that  $\psi_\varepsilon \rightarrow \psi$  in  $H^2(\mathbb{R}^{3N})$  and  $\psi_\varepsilon \rightarrow \psi$  uniformly on any compact set as  $\varepsilon \rightarrow 0$ , where the symbol  $*$  denotes the convolution of two functions. We introduce a strictly positive, continuous function defined by  $f_\varepsilon = \exp([\ln \psi_\varepsilon])$ . It is easy to see that  $f_\varepsilon$  also converges to  $f$  uniformly on any compact set, since, by the mean value theorem of calculus,  $|f_\varepsilon - f| \leq \text{const.} \cdot |\psi_\varepsilon - \psi|$  on any compact set. By direct computation, we see that

$$\Delta_i f_\varepsilon = (\Delta_i [\ln \psi_\varepsilon]) f_\varepsilon + |\nabla_i [\ln \psi_\varepsilon]|^2 f_\varepsilon \quad (2.1)$$

and  $\Delta_i [\ln \psi_\varepsilon] = [\Delta_i \ln \psi_\varepsilon]$  for  $i = 1, \dots, N$ , since  $[\Delta_N g] = [(\partial^2 / \partial r_N^2 + 2/r_N \partial / \partial r_N) g]$  for  $g \in C^2$ .

As  $\varepsilon \rightarrow 0$ ,  $\Delta_i f_\varepsilon$  converges to

$$F_i = \left( \left[ \frac{\Delta_i \psi}{\psi} \right] - \left[ \left| \frac{\nabla_i \psi}{\psi} \right|^2 \right] + |\nabla_i [\ln \psi]|^2 \right) f \quad (i = 1, \dots, N) \quad (2.2)$$

in  $L^1(K)$  for any compact set  $K \subset \mathbb{R}^{3N}$ . In fact, a simple calculation shows that

$$\left| \left[ \frac{\Delta_i \psi_\varepsilon}{\psi_\varepsilon} \right] f_\varepsilon - \left[ \frac{\Delta_i \psi}{\psi} \right] f \right| \leq \text{const.} (|\Delta_i (\psi_\varepsilon - \psi)| + |\psi - \psi_\varepsilon| |\Delta_i \psi| + |f_\varepsilon - f| |\Delta_i \psi|)$$

and

$$\begin{aligned} \left| \left[ \left| \frac{\nabla_i \psi_\varepsilon}{\psi_\varepsilon} \right|^2 \right] f_\varepsilon - \left[ \left| \frac{\nabla_i \psi}{\psi} \right|^2 \right] f \right| &\leq \text{const.} (|\nabla_i \psi_\varepsilon|^2 |f_\varepsilon - f| + [(|\nabla_i \psi_\varepsilon| + |\nabla_i \psi|) |\nabla_i \psi| |\psi_\varepsilon - \psi|] \\ &\quad + [(|\nabla_i \psi_\varepsilon - \nabla_i \psi| (|\nabla_i \psi_\varepsilon| + |\nabla_i \psi|)]) \end{aligned}$$

on any compact set. These bound and a similar calculation for the third term, together with  $f_\varepsilon \rightarrow f$  and  $\psi_\varepsilon \rightarrow \psi$  uniformly on any compact set and  $\psi_\varepsilon \rightarrow \psi$  in  $H^2(\mathbb{R}^{3N})$ , lead to the desired result (2.2).

Therefore, we obtain

$$\begin{aligned} \int_{\mathbb{R}^{3N}} f(x) \Delta_i \phi(x) dx &= \lim_{\varepsilon \rightarrow 0} \int_{\mathbb{R}^{3N}} f_\varepsilon(x) \Delta_i \phi(x) dx \\ &= \lim_{\varepsilon \rightarrow 0} \int_{\mathbb{R}^{3N}} \phi(x) \Delta_i f_\varepsilon(x) dx = \int_{\mathbb{R}^{3N}} \phi(x) F_i dx \end{aligned}$$

for any test function  $\phi \in C_c^\infty(\mathbb{R}^{3N})$ . Consequently, we learn  $F_i = \Delta_i f \in L_{\text{loc}}^1(\mathbb{R}^{3N})$  as the weak derivative. The proof of  $\nabla_i f \in L_{\text{loc}}^2(\mathbb{R}^{3N})$ , as the weak derivative, is virtually the same.

Finally, we note that  $|\nabla_N[\ln \psi_\varepsilon]|^2 = [(\partial/\partial r_N \psi_\varepsilon)/\psi_\varepsilon]^2 \leq [|\nabla_N \psi_\varepsilon|/\psi_\varepsilon]^2$  and  $|\nabla_i[\ln \psi_\varepsilon]|^2 \leq [|\nabla_i \psi_\varepsilon|/\psi_\varepsilon]^2$  for  $i = 1, \dots, N-1$ , by the Cauchy-Schwarz inequality. Then (2.1) implies that  $\Delta_i f_\varepsilon \leq [(\Delta_i \psi_\varepsilon)/\psi_\varepsilon] f_\varepsilon$ . Since  $\Delta_i f_\varepsilon$  converges to  $F_i = \Delta_i f$ , this yields

$$\begin{aligned} \int_{\mathbb{R}^{3N}} \phi \left[ \frac{\Delta_i \psi}{\psi} \right] f dx &= \lim_{\varepsilon \rightarrow 0} \int_{\mathbb{R}^{3N}} \phi \left[ \frac{\Delta_i \psi_\varepsilon}{\psi_\varepsilon} \right] f_\varepsilon dx \\ &\geq \lim_{\varepsilon \rightarrow 0} \int_{\mathbb{R}^{3N}} \phi \Delta_i f_\varepsilon dx = \int_{\mathbb{R}^{3N}} \phi \Delta_i f dx \quad (i = 1, \dots, N) \end{aligned}$$

for every non-negative test function  $\phi \in C_c^\infty(\mathbb{R}^{3N})$ .  $\square$

Using the decomposition

$$H_N^Z = H_{N-1}^Z - \Delta_N - \sum_{j=1}^K z_j |x_N - R_j|^{-1} + \sum_{i=1}^{N-1} |x_i - x_N|^{-1},$$

we observe that

$$\begin{aligned} 0 &= \left[ \frac{(H_N^Z - E_N^Z) \psi}{\psi} \right] f \\ &= \sum_{i=1}^{N-1} \left( - \left[ \frac{\Delta_i \psi}{\psi} \right] - \sum_{j=1}^K z_j |x_i - R_j|^{-1} \right) f + \sum_{1 \leq i < j \leq N-1} |x_i - x_j|^{-1} f \\ &\quad - \left[ \frac{\Delta_N \psi}{\psi} \right] f - \sum_{j=1}^K z_j [|x_N - R_j|^{-1}] f + \sum_{i=1}^{N-1} [|x_i - x_N|^{-1}] f - E_{N-1}^Z f. \end{aligned}$$

Here we have used the assumption  $E_N^Z = E_{N-1}^Z$ . Now we recall that our hypothesis  $Z = N-1$ , which gives us the bound

$$- \sum_{j=1}^K z_j [|x_N - R_j|^{-1}] + \sum_{i=1}^{N-1} [|x_i - x_N|^{-1}] \leq 0$$

in  $|x_N| > R = \max_{1 \leq j \leq K} |R_j|$ , since  $[|y - x_N|^{-1}] = \min(|y|^{-1}, |x_N|^{-1})$  for  $y \in \mathbb{R}^3$  by Newton's theorem (followed from an integration in polar coordinates). This is the crucial place where averaging over  $x_N$  helps.

We recall Lemma 2.1 to conclude that

$$0 \leq (H_{N-1}^Z - E_{N-1}^Z - \Delta_N) f$$

on  $|x_N| > R$ . In addition, by Zhislin's theorem and the HVZ theorem, there is a normalized eigenfunction  $\phi$  of  $H_{N-1}^Z$  corresponding to the eigenvalue  $E_{N-1}^Z$ . As in the case of  $\psi$ , we can assume that  $\phi > 0$ , etc. Thus, there is a sequence  $\phi_n \in C_c^\infty(\mathbb{R}^{3(N-1)})$  such that  $\phi_n \rightarrow \phi$  in  $H^2(\mathbb{R}^{3(N-1)})$  with  $\phi_n \geq 0$ . For any non-negative function  $\eta \in$

$C_c^\infty(\mathbb{R}^3)$  with the support in the set  $|x| > R$ , we define a non-negative, smooth, and compactly supported function by  $g_n(x_1, \dots, x_N) = \phi_n(x_1, \dots, x_{N-1})\eta(x_N)$ .

Lemma 2.1 now implies that

$$0 \leq \langle g_n, (H_{N-1}^Z - E_{N-1}^Z - \Delta_N) f \rangle = \langle (H_{N-1}^Z - E_{N-1}^Z - \Delta_N) g_n, f \rangle.$$

As  $n \rightarrow \infty$  the right side converges to  $\langle (H_{N-1}^Z - E_{N-1}^Z - \Delta_N) g, f \rangle$ , where  $g = \lim_{n \rightarrow \infty} g_n$ . Since  $H_{N-1}^Z \phi = E_{N-1}^Z \phi$ , it follows that

$$0 \leq \langle -\Delta_N g, f \rangle = \langle -\Delta \eta, v \rangle$$

for all  $0 \leq \eta \in C_c^\infty(\mathbb{R}^3)$  with the support in the set  $\{x : |x| > R\}$ , where

$$v(r_N) = \int_{\mathbb{R}^{3(N-1)}} \phi(x_1, \dots, x_{N-1}) f(x_1, \dots, x_{N-1}, r_N) dx_1 \cdots dx_{N-1}.$$

Hence, we find that  $v$  is superharmonic, that is,

$$0 \leq -\Delta v$$

on  $|x_N| > R$ , in distributional sense. Also,  $v_\varepsilon = h_\varepsilon * v$  is superharmonic in  $|x_N| > R + \varepsilon$  for sufficiently small  $\varepsilon > 0$ , where  $h_\varepsilon$  is some mollifier in  $\mathbb{R}^3$ . By the positivity of continuous functions  $f$  and  $\phi$ , we can choose a constant  $C_R > 0$  so that  $v_\varepsilon(x) \geq C_R |x|^{-1}$  for all  $x \in \mathbb{R}^3$  with  $|x| = R + 1$ . Since  $u(x) = C_R |x|^{-1}$  is harmonic in  $|x| > 0$ , we arrive at

$$-\Delta(u - v_\varepsilon) \leq 0 \quad \text{in } |x| > R + 1,$$

and by the strong maximum principle ([15, Theorem 9.4]), we learn that  $u - v_\varepsilon$  takes its maximum value on  $\{x \in \mathbb{R}^3 : |x| = R + 1\} \cup \{+\infty\}$ . Hence,  $\lim_{|x| \rightarrow +\infty} (u - v_\varepsilon)(x) \leq 0$  and  $u \leq v_\varepsilon$  on  $|x| = R + 1$  imply that  $u \leq v_\varepsilon$  in  $|x| > R + 1$ . From this result, we have  $u \leq \lim_{\varepsilon' \rightarrow 0} v_{\varepsilon'} = v$  for almost every  $x$  with  $|x| > R + 1$  and some subsequence  $\varepsilon'$ . Since  $C_R |x|^{-1} \leq v(x)$  for almost all  $|x| > R + 1$ , it immediately follows that

$$\int_{\mathbb{R}^3} v(r_N)^2 dx_N = +\infty.$$

From the fact that  $f \leq [\psi]$  (recall the first line of the proof of Lemma 2.1) and the Cauchy-Schwarz inequality, we conclude

$$\begin{aligned} +\infty &= \int_{\mathbb{R}^3} v(r_N)^2 dx_N \\ &= \int_{\mathbb{R}^3} \left( \int_{\mathbb{R}^{3(N-1)}} \phi(x_1, \dots, x_{N-1}) f(x_1, \dots, x_{N-1}, r_N) dx_1 \cdots dx_{N-1} \right)^2 dx_N \\ &\leq \int_{\mathbb{R}^{3N}} f(x_1, \dots, x_{N-1}, r_N)^2 dx_1 \cdots dx_N \leq \int_{\mathbb{R}^{3N}} [\psi]^2 dx_1 \cdots dx_N \leq \|\psi\|_2^2. \end{aligned}$$

This contradicts to  $\psi \in L^2(\mathbb{R}^{3N})$ .

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